Bisphenol A

80-05-7 | DTXSID7020182

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 2.74

Global applicability domain: Inside

Local applicability domain index: 5.43e-01

Confidence level: 5.28e-01

Nearest Neighbors from the Training Set

Image not found
Ethyl 1-naphthaleneacetate
Measured: 2.48
Predicted: 2.63

Image not found
Isopropylpropyzamide
Measured: 2.17
Predicted: 2.24

Image not found
3,3'-Dichlorobenzidine
Measured: 4.35
Predicted: 3.23

Image not found
N-Cycloheptyl-N'-phenylurea
Measured: 2.37
Predicted: 2.34

Image not found
Carboxin
Measured: 2.41
Predicted: 2.32